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Abstract

The desired shifts of the boundaries of spectral allowed zones of periodical systems are demonstrated. In particular, the phenomenon of merging neighbor allowed zones is exhibited and its simple explanation is given. It is also shown how to change the additional fundamental spectral parameter, the degree of exponential solution growth, at arbitrary given energy points inside the forbidden zones. This allows one to control tunneling through fragments of periodic structures at energies belonging to spectral gap. All the results are based on the finite interval **inverse** eigenvalue problem which provides us with *complete sets* of exactly solvable models. This is a radical extension (continuous ! multiplicity) in comparison to the famous finite-gap models.

PACS numbers: 03.65.-w; 02.30.Zz

The periodical structures represent an area of intensive research and diverse practical applications, e.g., in microelectronics. So it is important to extend as far as possible the class of spectral zone control algorithms. We suggest, in particular, potential transformations leading to given shifts of chosen zone boundaries.

We apply our experience (quantum intuition) in the *finite interval* inverse problem (IP) algorithms [1-4], which allow the construction of the potentials corresponding to a given set of spectral parameters, e.g., bound state energy levels and spectral weights $\{E_\lambda, c_\lambda\}$, *to periodic case.* In the IP formalism [5-8] these parameters are input parameters uniquely determining the potential and so can be considered as spectral "control levers". Corresponding **exact models form the complete sets**. The next step is the periodical continuation over the whole axis the potential derived with the inversion procedure on finite interval. So we use the missed possibility to combine *inverse* problem approach on a finite interval with *direct* one of constructing solutions for the periodically continued potential (infinitely enriched Kronig-Penney-like procedure). This gives us additional flexibility of the formalism in comparison with the *pure inverse* finite gap theory of spectral band structures.

Let us use, for example, the formulae for energy level shift in infinite rectangular potential well of finite width. Let $\psi_0(x, E_n)$ be corresponding eigenfunction at the energy E_n. We assume $\bar\psi_0(x, E_n + t)$ to be a non-physical auxiliary solution in the initial potential at the shifted energy $E_n + t$ with the symmetry being opposite to one of the $\psi_0(x, E_n)$. With these solutions, we can construct the Wronskian

$$\begin{aligned} \theta(x) &= \psi_0'(x, E_n)\bar\psi_0(x, E_n + t) \\ &\quad -\psi_0(x, E_n)\bar\psi_0'(x, E_n + t). \end{aligned} \tag{1}$$

The final expressions for the transformed potential and solutions are

$$V_2(x) \quad = \tag{2}$$

$$V_0(x) - 2\,t\,\frac{d}{dx}\{\psi_0(x,E_n)\bar{\psi}_0(x,E_n+t)\theta(x)^{-1}\}; \tag{3}$$

$$\psi(x,E) = \psi_0(x,E) - \tag{4}$$

$$t\bar{\psi}_0(x,E_n+t)\theta(x)^{-1}\int^x \psi_0(y,E_n)\psi_0(y,E)dy; \tag{5}$$

$$\psi(x,E_n+t) \quad = \quad \psi_0(x,E_n)\theta(x)^{-1}. \tag{6}$$

It appears that our ability to shift isolated bound state energy levels (over the E-scale) in the infinite potential well on a finite interval allows us to move some chosen upper (lower) boundaries of the spectral zones (bands) of periodic structures keeping infinite number of other upper (lower) boundaries unperturbed.

Let us consider instructive particular examples. The above formulae can be periodically continued and used for spectral control of the initial Dirac comb (equidistant δ-potential barriers or wells $\sum_{m=-\infty}^{\infty} \overset{\circ}{V}\ \delta(x-m\pi)$. To be more precise, we get the following periodic potential: $\sum_{m=-\infty}^{\infty} \overset{\circ}{V}\ \delta(x-m\pi) + V^{per}(x),\ \ V^{per}(x+l\pi) = V_2(x),\ \ l = 0;\pm1;\pm2;....$ In Fig.1a transformations of spectral zones in the case $\overset{\circ}{V}= 4$ corresponding to the successive shifts up of second level $\overset{\circ}{E}_2= 4 \rightarrow E = 9$ of the auxiliary problem are demonstrated. Pay attention to the merging of the second and third allowed zones at special value of $\Delta E = 1$ and their separating after further moving E_2 up.

It is remarkable that at first ($\Delta E \leq 1$) the lower boundary of the upper neighbor allowed zone goes down to meet the approaching level E_2 until the second and the third allowed zones merge.

Compare it with the opposite situation on (in) Fig.1b when E_2 is shifted down, moving away from the third level. Then the zone below the fixed level E_3 shrinks and goes up until its complete disappearance. The second zone at $\Delta E = -1.8$ merges with the first zone and after that the first zone recoils down.

These points of zone junction are especially interesting. The phenomenon of zone merging can be clarified if we consider the continuous transformation of Dirac comb with δ-barriers into one with δ-wells. In the first case the allowed zones have the auxiliary levels as upper boundaries and in the second as lower ones [9]. For zero V_δ all the gaps between zones disappear while transiting from repulsion to attraction. Then the auxiliary levels E_n are simultaneously upper boundaries for the upper nth allowed zones and lower boundaries for the lower $n-1$th zones and there is the continuous spectrum from $E = 0$ to $E \rightarrow \infty$. This allows us to suppose that in the case of non-zero potentials there is "balance" between attraction and repulsion only in the vicinity of E-point of zone junction where the E_2 level becomes a "boundary" for both neighbor zones.

When shifting E_2 further upward there occurs the transition to the regime of a local prevalence of the attraction and E_2 ceases being the upper boundary of the second zone. This zone separates from its previous upper boundary E_2 and recoils downward.

The reappearance of the vanished gap between 2nd and 3rd zones can be explained as follows. During the further shifting the E_2 level up through the balance point, the local predominance of repulsion is changed by the prevalence of attraction. So the level E_2 becomes only the lower boundary of the upper zone abandoning the lower zone which moves down restoring the just disappeared gap. The same effects can be observed in Figs.1a,c.

Let us shift auxiliary energy levels starting from free motion without Dirac combs (continuous spectrum with all gaps collapsed). Then the experience we have already got allows one to predict the qualitative zone movement. For this it would be useful consideration of right sides of Figs.1a-c after the first zone merging.

Now we shall consider another example of zone control. Below are given the formulas for the potential and wave functions transformations corresponding to variations of spectral weight factor c_n of a chosen bound state at the energy E_n (see a general case in [1, 2, 10]): Let $\overset{\circ}{\psi}_m(x)$ be an eigenfunction of the initial Hamiltonian corresponding to mth energy eigenvalue, $\overset{\circ}{c}_m$'s are the initial spectral weight factors. Then changing $\overset{\circ}{c}_m \rightarrow c_m$ gives

$$\psi_n(x) = \overset{\circ}{\psi}_n(x) + \frac{(1 - c_m^2/\overset{\circ}{c}_m{}^2)\,\overset{\circ}{\psi}_m(x)}{1 - (1 - c_m^2/\overset{\circ}{c}_m{}^2)\int_0^x \overset{\circ}{\psi}_m{}^2(y)dy} \times \int_0^x \overset{\circ}{\psi}_m(y)\,\overset{\circ}{\psi}_n(y)dy, \tag{7}$$

$$V(x) = \overset{\circ}{V}(x) + 2\frac{d}{dx}\frac{(1 - c_m^2/\overset{\circ}{c}_m{}^2)\,\overset{\circ}{\psi}_m{}^2(x)}{1 - (1 - c_m^2/\overset{\circ}{c}_m{}^2)\int_0^x \overset{\circ}{\psi}_m{}^2(y)dy}. \tag{8}$$

The transformed solution $\psi_n(x)$ differs from the initial one by that varying the parameter c_n changes the space distribution of wave function (localization) [11, 12, 13].

We need not restrict ourselves to the discret spectral points of the auxiliary infinite rectangular well and zero boundary conditions at its walls. In usual periodical problems there are no impenetrable walls. So, arbitrary homogeneous boundary conditions apply for our goals. Corresponding corrections for the above formulas can be easily derived [1, 2]

It turns out that the algorithms of shifting localization of eigenfunctions over the configurational axis x result in changing the degree of forbiddenness of the spectral gap at the chosen energy point, see Fig.1d. It can be easier understood in the case of symmetrical initial potentials with the (anti)symmetrical eigenfunctions. Then variation of c_n violates the symmetry which results in exponential growth of the periodically continued solution swinging. This is peculiar to the forbidden zone. The more the change in c_n the greater the degree of forbiddenness (i.e., c_n is a 'lever' of direct control). The same is true for the general boundary conditions, i.e., arbitrary energy point in the forbidden zone. In particular, this drastically ('continuous' multiplicity) extends the class of exactly solvable models, which may be of great value in clarifying different aspects of periodic system theory.

The transformations based on shifting a chosen energy level E^I_μ in one of two auxiliary spectra corresponding to the same system are equivalent to changing infinite spectral weight factors of another spectrum, e.g., increasing $c^{II}_n; n > \mu$ and decreasing $c^{II}_n; n < \mu$ [14]. We have not still analyzed the influence of such shifts on band spectral structure.

Just before the submission of this paper we revealed unexpected symmetry. The shifts of "nonphysical" levels $E \to E \pm \Delta E$ in the infinite rectangular well give the same deformation (we started from free motion) of the band structure of the periodically continued potential for arbitrary ΔE and E, which does not violate the rule: no crossing the levels of the physical spectrum while shifting energy level. It is an intriguing open problem to explain the phenomenon of coincidence of band structures for different periodic potentials, which (up to our knowledge) was never mentioned before.

Conclusions – New status of quantum mechanics is due to achievements of the inverse problem approach [1, 2]. Instead of about ten exactly solvable models which serve as a basis of the contemporary research and education there are infinite (!) number, even **complete** sets of such models. So, the whole quantum mechanics is embraced by them. They correspond to all possible variations of spectral parameters which determine all properties of quantum systems. There appears a possibility to change at wish quantum objects by variation of these parameters as control levers and examine quantum systems in different thinkable situations. The regularities revealed by computer visualization of these models were reformulated into unexpectedly simple universal rules of arbitrary transformations and what is more, their elementary constituents were discovered. Of these elementary 'bricks' it is possible in principle to construct objects with any given properties. The embedding of potentially real objects into the continuum of all the thinkable exactly solvable models allows to unify the whole picture, gives a notion of the connections between the systems considered before as completely different ones. This simplifies the science and gives a significant economy of memory to be used for our further creative activity.

The well-known finite-gap potentials [5, 6] might serve as a good example of corresponding exact models. At the same time these potentials have the obvious fault that they are not flexible enough: they have 'frozen' distribution of forbiddeness index.

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FIGURE CAPTIONS

Fig.1a Shifting up the upper boundary of the second allowed zone for the Dirac comb (periodical δ-barriers). This boundary coincides with the second energy level in the auxiliary well with impenetrable walls at the ends of finite period interval. It pools at first its zone while moving upward. And the lower boundary of the neighbor upper 3rd zone is lowering toward it until at $\Delta E = 1$ both neighbor zones merge. The second energy level of the transforming auxiliary well becomes the lower boundary of the upper zone at this moment. After that the zones are separating again $\delta E = 2, 3, 3.9$, but the shifted level now remains with the upper zone. Its motion up squeezes the upper zone (between two levels) until annihilation, because its upper boundary $E = 9$ remains unchanged according to the algorithm of shifting the only one energy level.

Fig.1b Shifting down the upper boundary of the 2nd allowed zone of the Dirac comb of δ-barriers. This boundary pushes downward the 2nd zone before it until its lower boundary touches the lower first allowed zone which fixed boundary $E = 1$ becomes at this moment also the lower boundary of the zone coming from above. After the zone merging the lower zone separates from the upper one and goes downward while the upper zone is squeezed between its boundaries: the fixed $E = 1$ and lowering second energy level of the auxiliary well.

Fig.1c Shifting up the lower boundary of the second allowed zone of Dirac comb δ-wells (ground state of the auxiliary eigenvalue problem on the period). This boundary pushes the zone upward from below until its upper boundary achieves the second fixed energy level $E = 4$. At this moment the spectral gap between the two zones disappears. After that the squeezing of the lower zone begins similarly to the case of Fig.2. Simultaneously, the upper zone separates and goes upward restoring the just disappeared lacuna. The degeneration of auxiliary energy levels is followed by their effective annihilation [2, 13] and by the collapse of all the allowed zones.

Fig.1d (upper part) Changes in zone structure corresponding to relative variations of spectral weight factors $c/ \overset{\circ}{c}$ at energy point $E = 2$. The initial periodic potential $\overset{\circ}{V} \delta(x - n\pi)$ has Dirac comb peaks with the strength $\overset{\circ}{V} = 4$ and period π. The wave function at $E = 2$ is on each period an eigenfunction of the eigenvalue problem with the boundary conditions on the edges of a period specified so that the auxiliary discrete energy level just coincides with the chosen point $E = 2$. (Lower part) Changes of the imaginary part of quasi-momentum $ImK(E)$ which characterize the degree of forbiddeness, the index of exponential swinging of solutions.